CEMHYD3D: Overview and Current Status

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Model Characteristics

- Three-dimensional (100 µm on a side)
- Multi-size, multi-phase cement particles
  – representative of real cement of interest
- silica fume, fly ash (future- slag, kaolin)
- gypsum, hemihydrate, and/or anhydrite sulfate sources
- simulates dissolution, diffusion, & reaction

Inputs to CEMHYD3D

- Cement (mineral admixture) particle size distribution
- cement bulk composition and surface composition
- apparent activation energies for cement and mineral admixtures
- volume fraction of aggregates
- curing conditions
  - isothermal/ adiabatic/ temperature profile
    - maturity method principles
  - saturated/ sealed/ drying
    - self-desiccation and creation of "empty" porosity

Outputs from CEMHYD3D

- Degree of hydration vs. time
  – all phase volume fractions
- chemical shrinkage vs. time
- heat release vs. time
  – adiabatic heat signature
- compressive strength (Power's gel-space ratio)
- diffusivity (w/c, α, V_{agg}, M_{SF})
- percolation of porosity (CH) -- durability
- percolation of solids -- setting
- ITZ microstructure
  - phase fractions vs. distance from aggregates

Model Usage

- Academia (education and Ph. D. research)
  - U.S. (ACBM, UC Berkeley, Georgia Tech, Tennessee Tech)
  - France (Cachan)
  - The Netherlands (Twente)
  - Denmark (Technical University of Denmark)
  - Japan (Tokyo Institute of Technology)
  - China
  - South Africa (Capetown)

Model Usage

- Industry
  - Germany (Dyckerhoff Zement)
  - France (CSTB)
  - The Netherlands
- Government
  - Waterways Experiment Station

Studies to Date Using Model

- Calibration/Prediction studies
  - heat release and adiabatic heat signature
  - degree of hydration
  - chemical shrinkage
  - compressive strength
- Effects of cement PSD on properties
  - coarser cements for low w/c ratio concretes
  - early age autogenous properties and cracking

Heat of Hydration

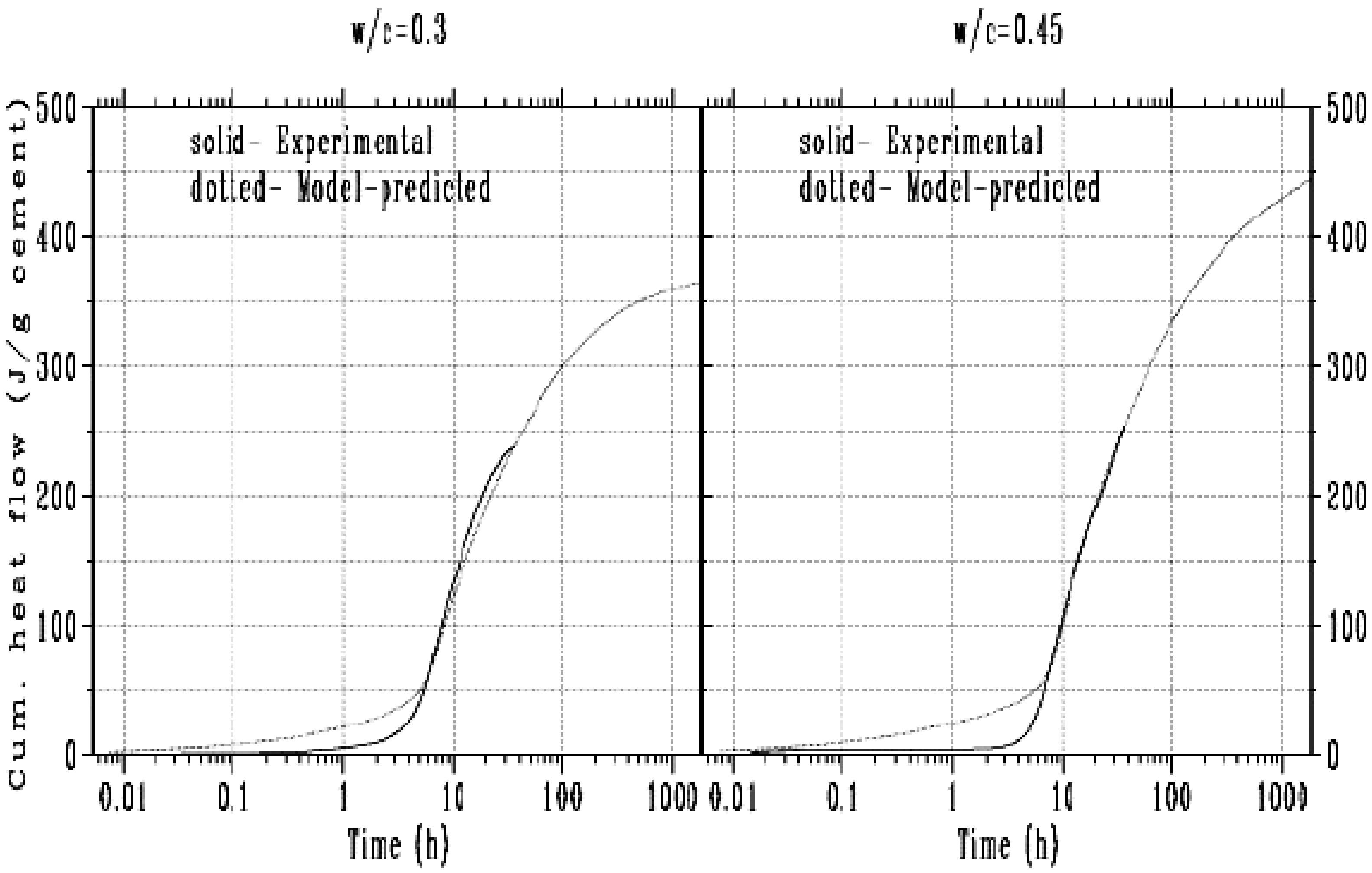
- Determine heat of hydration by monitoring how much of each phase reacts/forms during each cycle
- Base results on heats of formation of each compound or on **measured heats of hydration of phases**

Compound	Heat of Hydration
C_3S	517 J/g
C_2S	262 J/g
C_3A	1144 J/g
C_4AF	725 J/g

– Taylor, H.F.W., Cement Chemistry, 1992.

– Fukuhara et al., *Cem Concr Res*, **11**, 407-414, 1981.

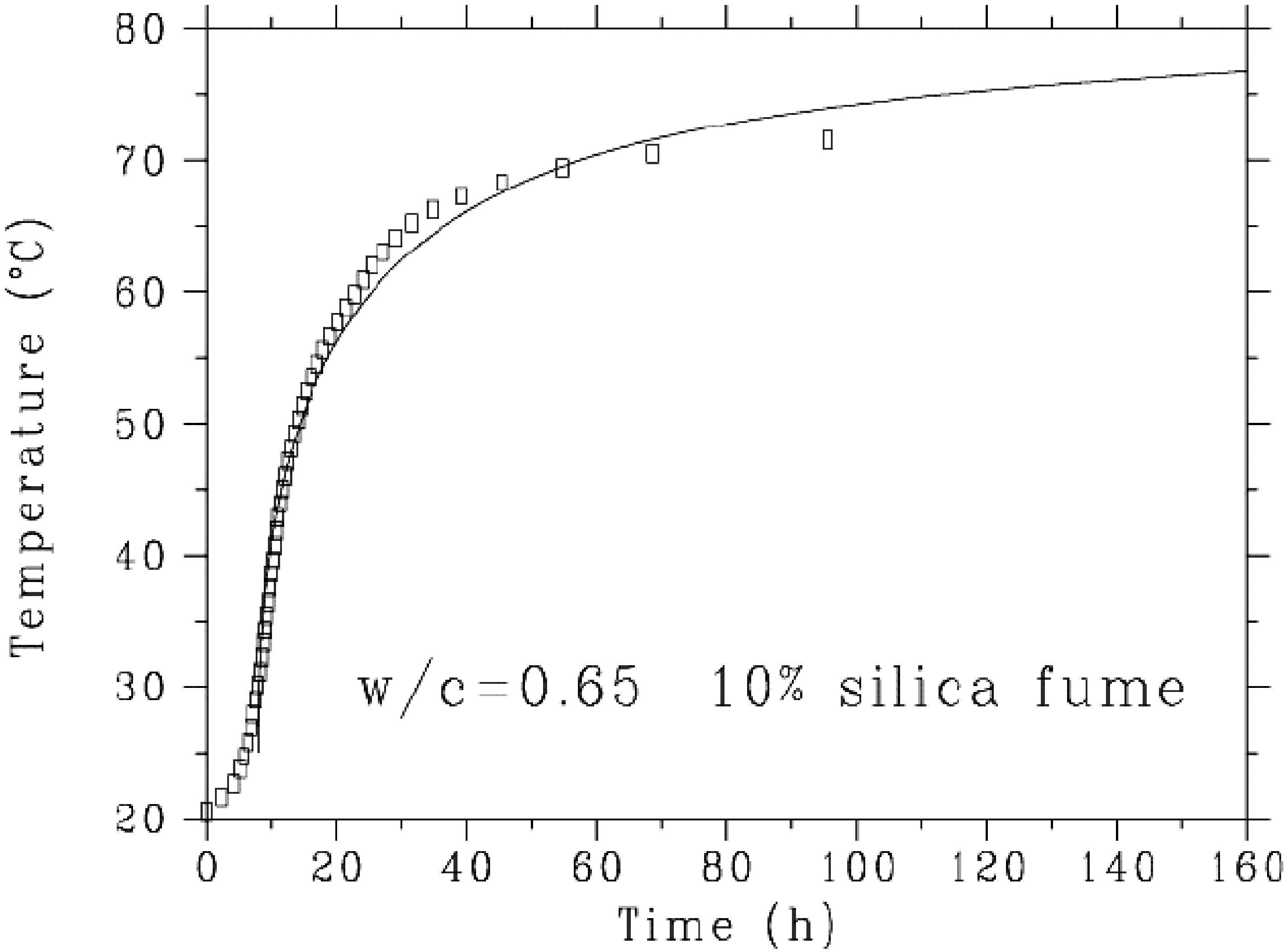
Heat of hydration



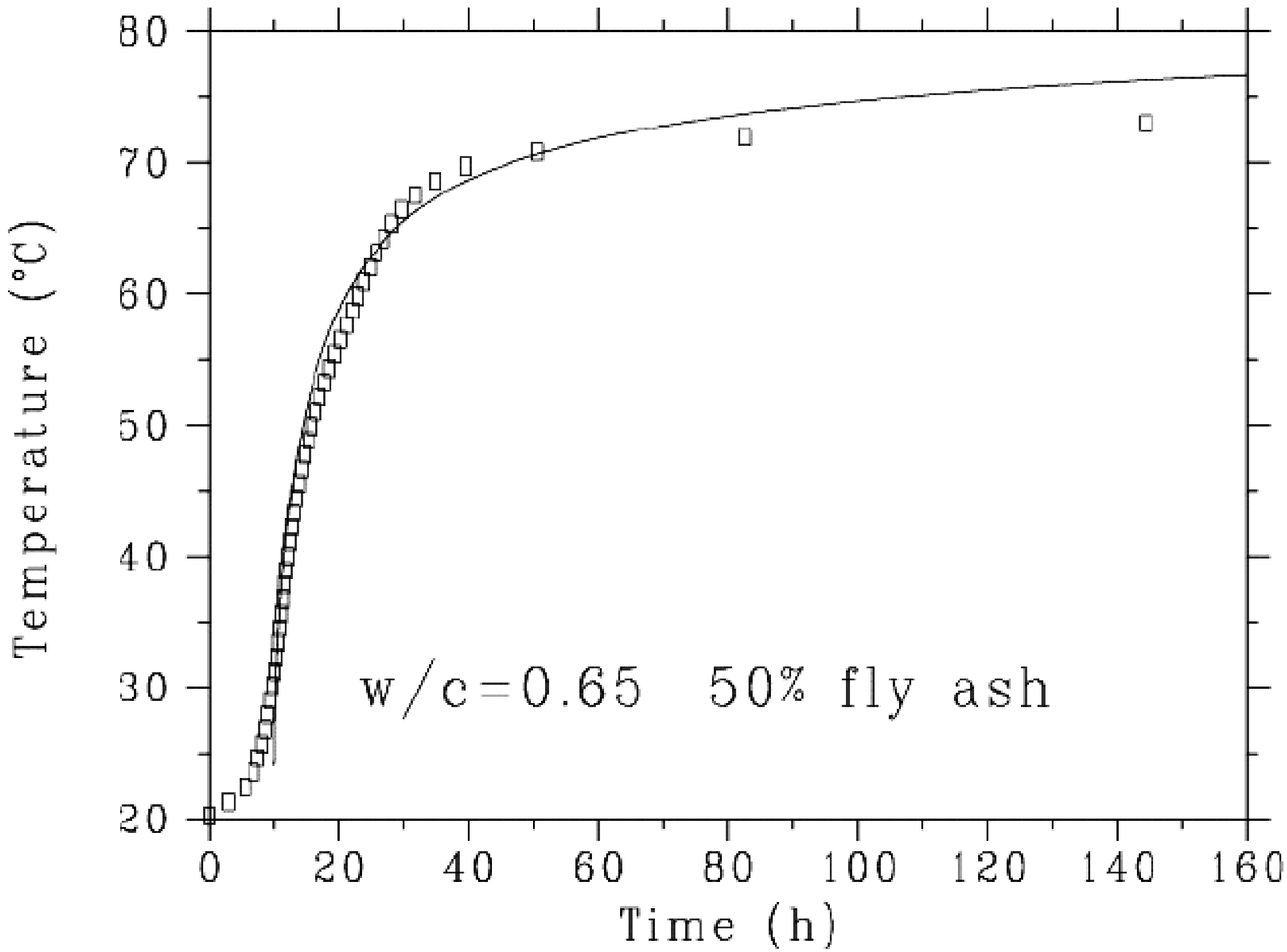
Temperature Calculation for Adiabatic Conditions

- Update heat released and heat capacity after each cycle of hydration model and calculate T rise via:
  - $\Delta T = [H(I)-H(I-1)]/C_p(I)$
    - H(I) is heat released through cycle I
      - H(I) is based on heats of reaction of clinker phases
    - $C_p(I)$ is heat capacity of concrete after cycle I
      - heat capacity adjusted for imbibition of water into cement paste and conversion of free to bound water

Predicted Adiabatic Heat Signature



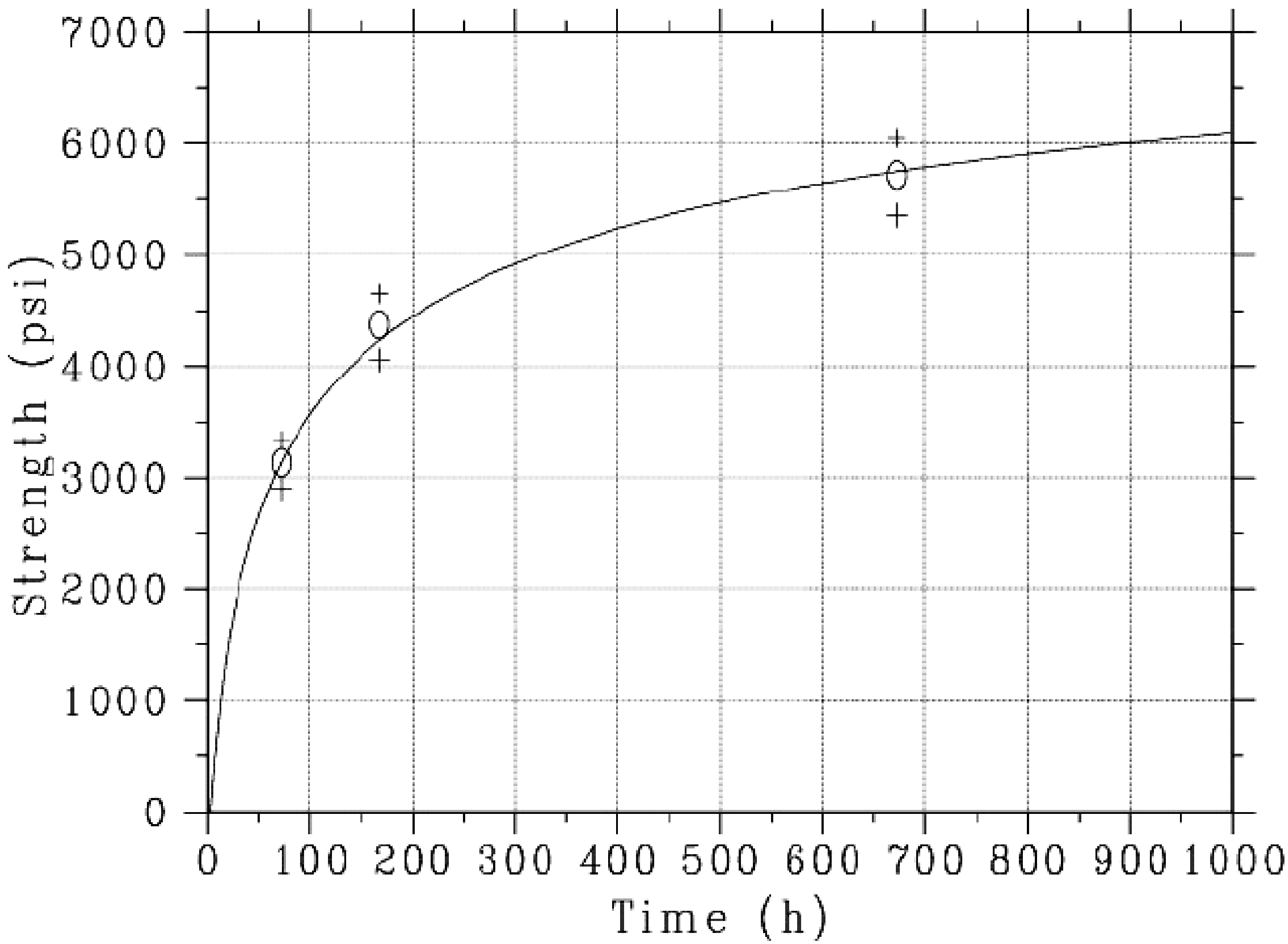
Predicted Adiabatic Heat Signature



Prediction of Compressive Strength

- Use gel-space ratio theory of Powers and Brownyard
  - $X = (0.68 * \alpha)/(0.32 * \alpha + w/c)$
  - $\sigma_c = A * X^n$ (n=2.6 to 3.0)
- Calibrate A via measured 3-day compressive strength (assume n=2.6)
- Use hydration model to predict X vs. time and calculate 7-day and 28-day compressive strengths to compare to experiment

Compressive Strength Prediction



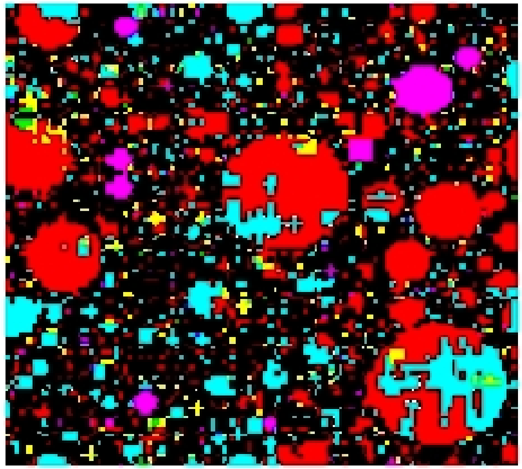
Cement PSD and Properties

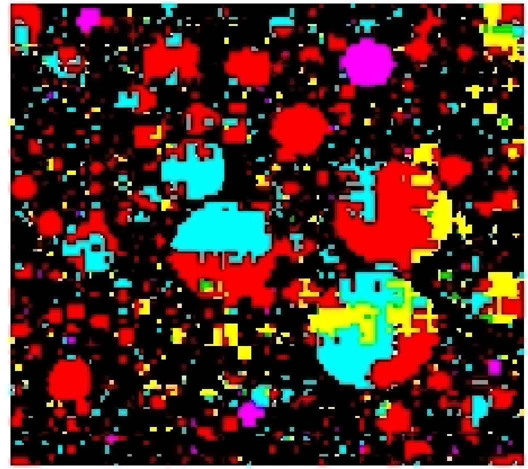
- Cement finenesses have increased dramatically from the 1950's (250-300 m^2/kg) to present date (350-400 m^2/kg)
- High performance concrete mixture proportions substantially different from conventional ones (lower w/c ratio, silica fume, etc.)
- Question: Have cements been optimized for HPC mixture proportions? --> CEMHYD3D

Systems Examined

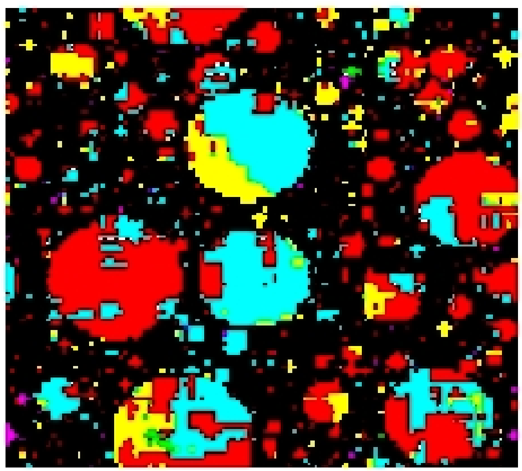
- Clinker ground to different finenesses
  - <5 µm> 643 m^2/kg <10 µm> 520 m^2/kg
  - <15 µm> 387 m^2/kg <20 µm> 296 m^2/kg
  - <25 µm> 254 m^2/kg <30 µm> 212 m^2/kg
- Composition: C_3S- 56.3 %, C_2S- 24.7 %, C_3A- 0.6 %, C_4AF- 13.5 %, Hemi- 4.6-5 %

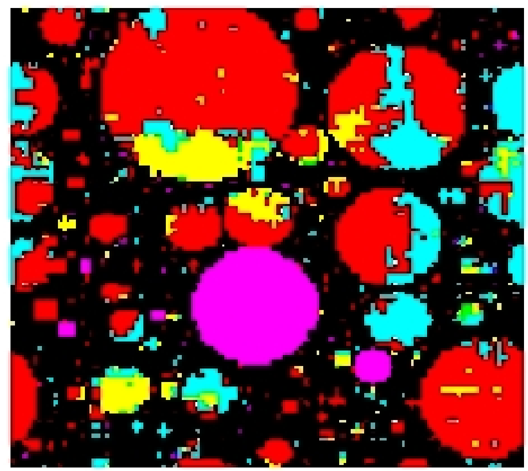
2-D slices from initial 3-D cement microstructures





643 m*m/kg   w/c=0.35   387 m*m/kg





254 m*m/kg   212 m*m/kg

Note the increase in particle spacing (pore size) for the two coarser cements (254 and 212)

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

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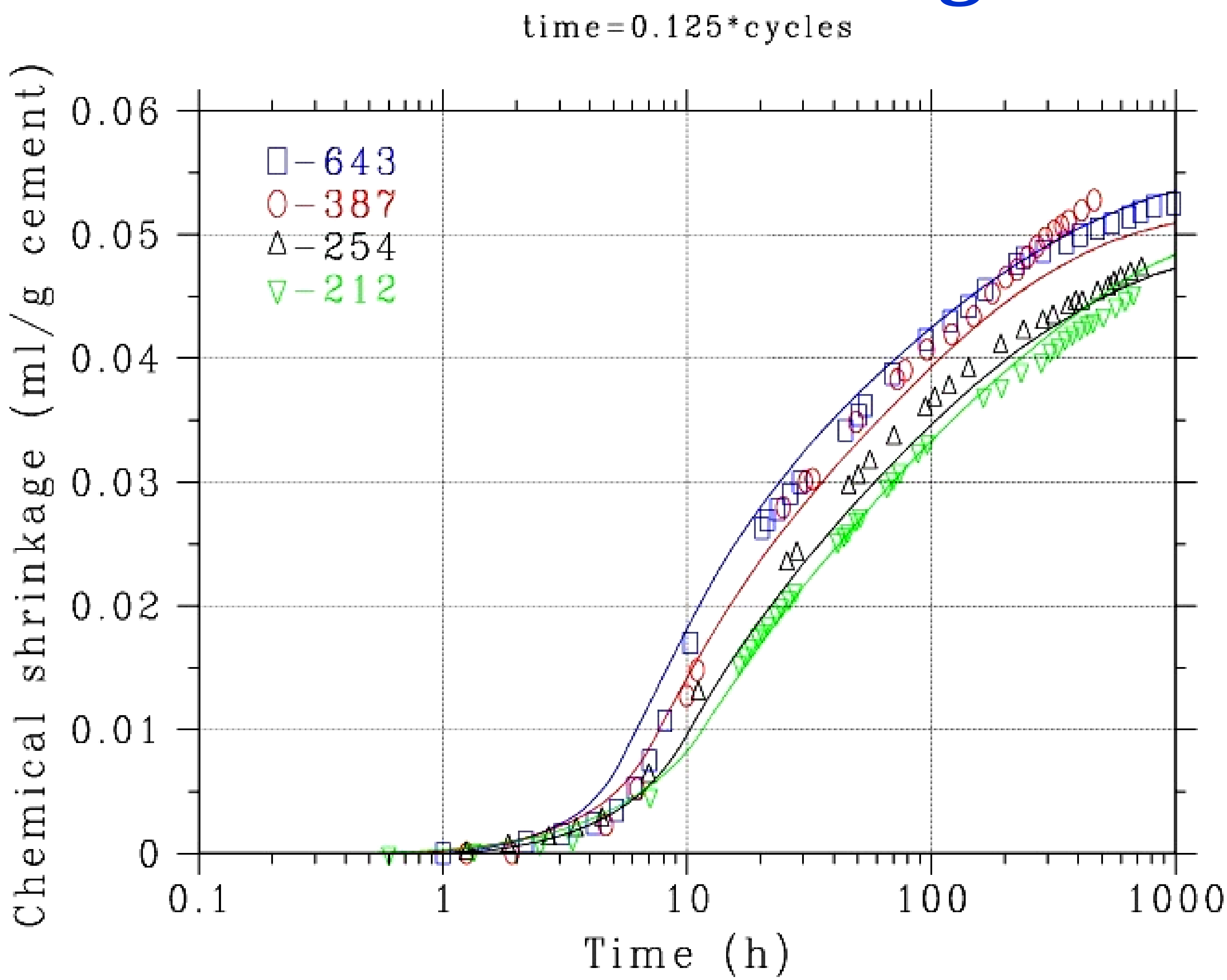
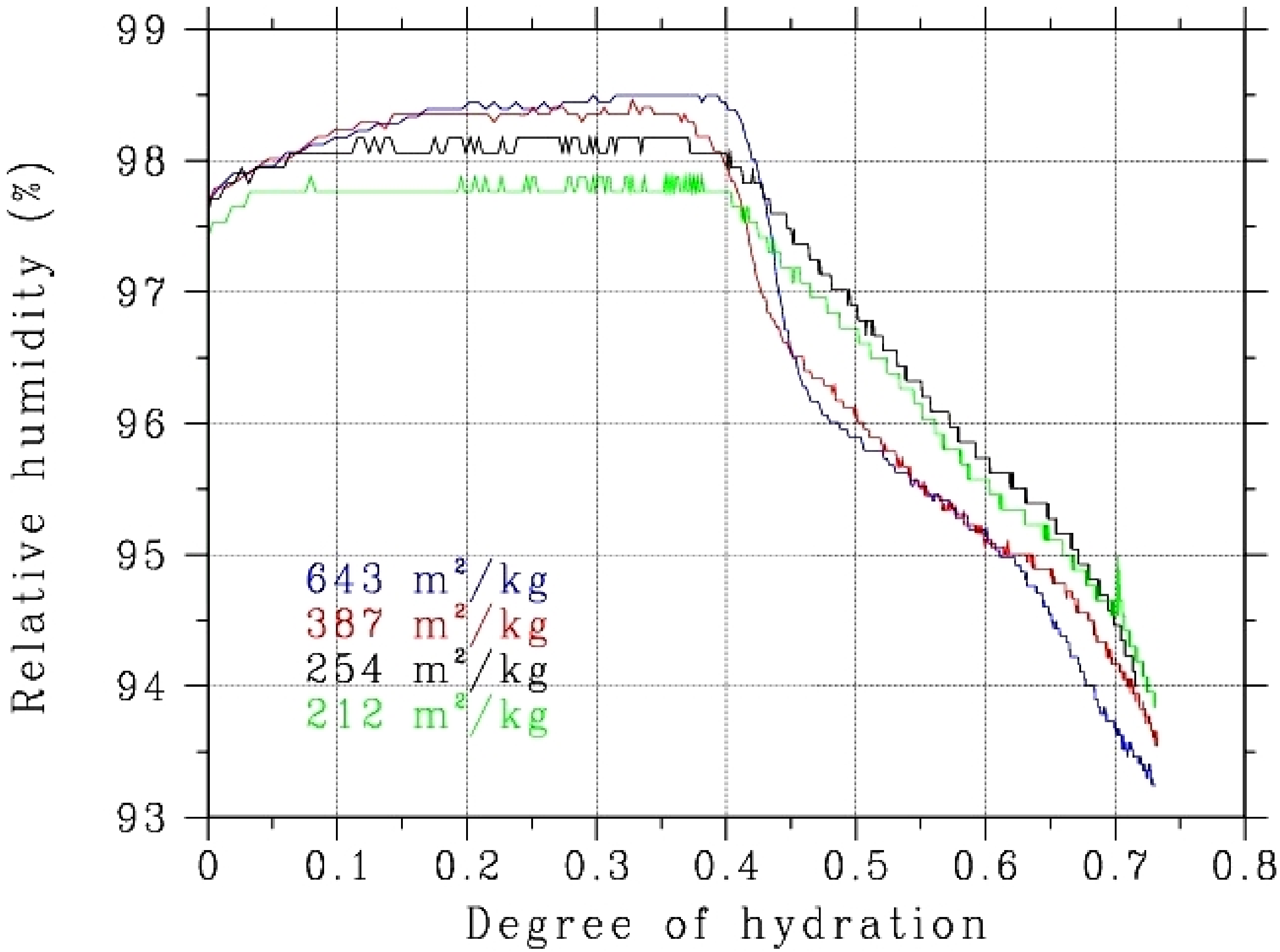
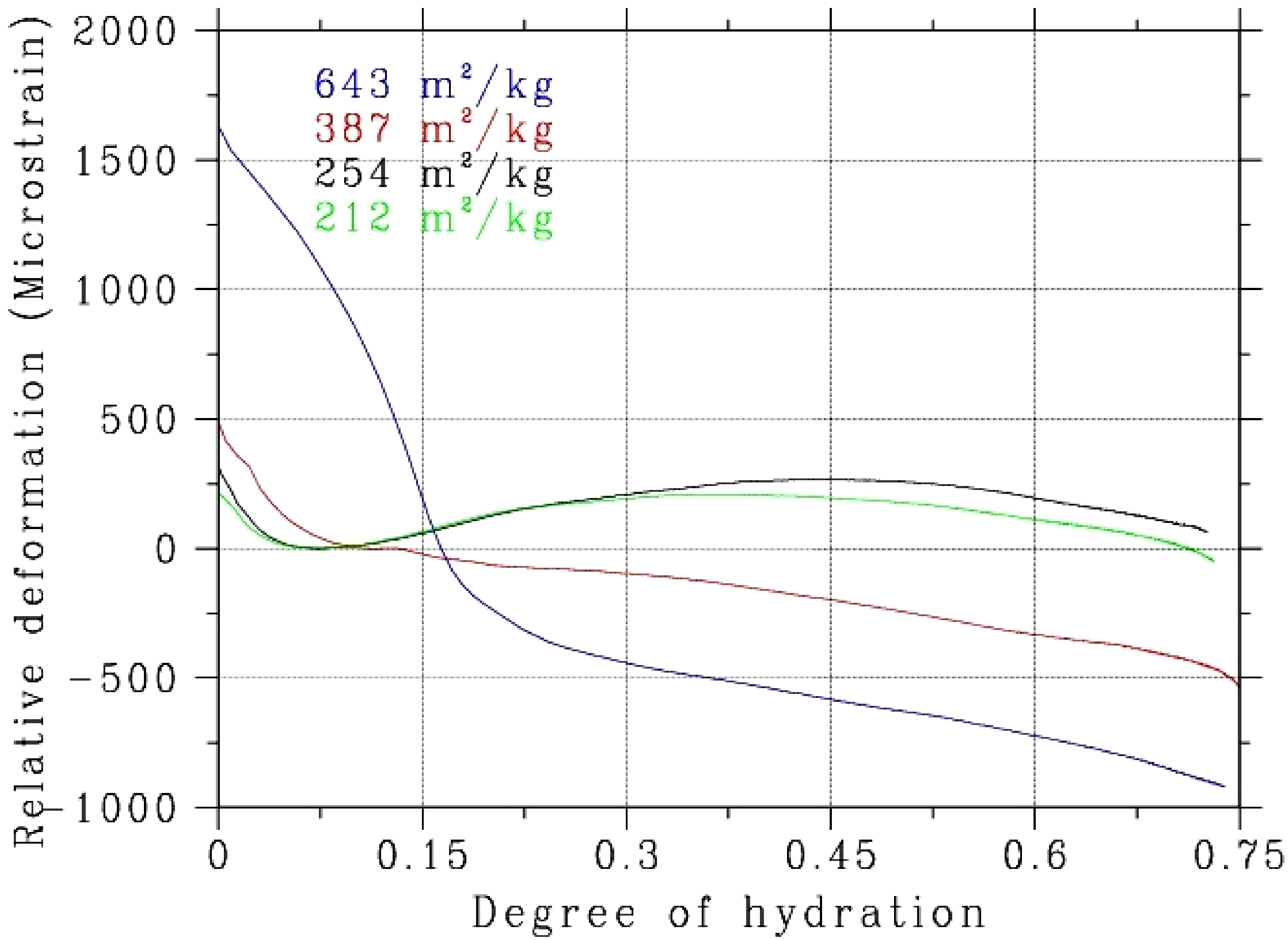
Chemical Shrinkage



Internal Relative Humidity



Autogenous Shrinkage



Conclusions

- In HPCs, coarser cements:
  - reduce early hydration and heat release (and strength!)
  - enhance “curability” by shifting depercolation of capillary porosity to lower values
  - increase diffusivities at early times, but result in equivalent diffusivities at longer times (equivalent hydration)
  - reduce internal RH reduction and autogenous strains and stresses

What's missing?

- Better modeling of influence of sulfate
  - work in progress with Dyckerhoff Zement
- Modeling of influence of alkalies
  - some work done for a Ph. D. in The Netherlands
- Modeling of slag, kaolin, others
  - ongoing experimental studies to clarify mechanisms and reactions
- Modeling of influence of specific chemical admixtures
- ……………………………....